

# Heat Flow in Classical and Quantum Systems and Thermal Rectification

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**Abstract.** The understanding of the underlying dynamical mechanisms which determine the macroscopic laws of heat conduction is a long standing task of non-equilibrium statistical mechanics. A better understanding of the mechanism of heat conduction may lead to potentially interesting applications based on the possibility to control the heat flow. Indeed, different models of thermal rectifiers has been recently proposed in which heat can flow preferentially in one direction. Although these models are far away from a prototype realization, the underlying mechanisms are of very general nature and, as such, are suitable of improvement and may eventually lead to real applications. We briefly discuss the problem of heat transport in classical and quantum systems and its relation to the chaoticity of the dynamics. We then study the phenomenon of thermal rectification and briefly discuss the different types of microscopic mechanisms that lead to the rectification of heat flow.

**Keywords:** Heat transport, Nonlinear dynamics and chaos, Quantum chaos, Nonequilibrium thermodynamics

**PACS:** 05.70.Ln, 05.45.Mt, 44.10.+i

## INTRODUCTION

The origin of the macroscopic phenomenological laws of transport is still one of the major challenges in theoretical physics. In particular, the issue of heat transport, in spite of having a long history, is not completely settled [1, 2]. Given a particular classical, many-body Hamiltonian system, neither phenomenological nor fundamental transport theory can predict whether or not this specific Hamiltonian system yields an energy transport governed by the Fourier law  $J = -\kappa \nabla T$ , relating the macroscopic heat flux to the temperature gradient  $\nabla T$  [3].

In spite of intense investigations in recent years, [4, 5, 6, 7, 8, 9, 10, 11, 12, 13] the precise conditions that a dynamical system of interacting particles must satisfy in order to obey the Fourier law of heat conduction are still not known. However, the general picture that emerges is that, for systems with no globally conserved quantities (i.e., globally ergodic), positive Lyapunov exponents is a sufficient condition to ensure the Fourier heat law.

Given the state of affairs, a common strategy is to investigate up to what extent one can simplify the microscopic dynamics and yet obtain a normal transport behavior. Thermal transport has been studied for a Lorentz channel –a quasi-one-dimensional billiard with circular scatterers– and it was shown to obey the Fourier law [8], yet we do not have rigorous results and in spite of several efforts, the connection between Lyapunov expo-

nents, decay of correlations and diffusive and transport properties is still not completely clear. For example, in a recent paper [9], a model was presented which has zero Lyapunov exponents, yet it exhibits unbounded Gaussian diffusive behavior. Since diffusive behavior is at the root of normal heat transport, the above result constitutes a strong suggestion that normal heat conduction can take place even without the strong requirement of exponential instability. The models in Refs. [8] and [9] are noninteracting: thus, the condition of Local Thermal Equilibrium (LTE) is not satisfied.

At the quantum level, the question whether normal transport may arise from the underlying quantum dynamics remains an open issue [14, 15]. This is mostly because it is not clear how to describe the transport of energy or heat from a microscopic point of view. In analogy to classical systems, a quantum derivation of the Fourier law calls directly in question the issue of quantum chaos [16]. However, a main feature of quantum motion is the lack of exponential dynamical instability [17]. This fact may render very questionable the possibility to derive the Fourier law of heat conduction in quantum mechanics. Thus it is interesting to inquire if, and under what conditions, Fourier law emerges from the laws of quantum mechanics (for a recent review of the microscopic foundations of the quantum Fourier law see [18]).

In this paper we present a brief review of heat transport in classical and quantum systems. We then investigate the possibility to control the energy transport and discuss different microscopic mechanical models in which thermal rectification can be observed. The possibility of controlling heat conduction by nonlinearity opens the way to design a thermal rectifier, *i.e.*, a system that carries heat preferentially in one direction while it behaves as an insulator in the opposite direction.

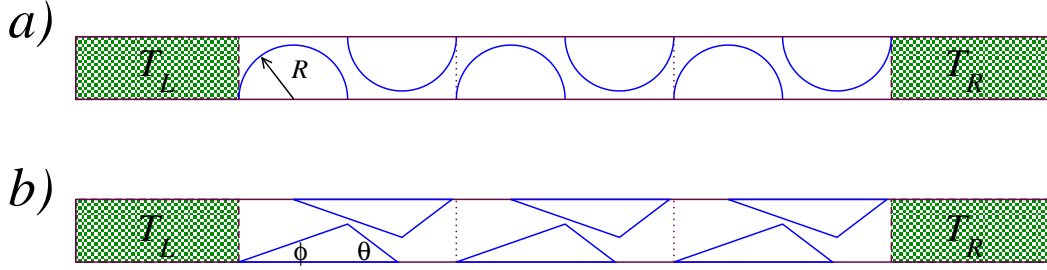
## **DYNAMICAL INSTABILITY AND FOURIER LAW**

### **Fourier Law in Classical Systems**

To clarify the role of dynamical instability for the validity of Fourier law, different microscopic mechanical models (*e.g.*, chains of anharmonic oscillators and billiards) have been investigated. Here we focus on billiards with integrable or chaotic dynamics.

Motivated by the ergodicity and mixing properties of the Lorentz gas, in Ref. [8] a channel geometry has been considered to study the problem of heat conduction in this model. A Lorentz gas consists of noninteracting point particles that collide elastically with a set of circular scatterers on the plane (see Fig. 1-*a*). By imposing an external thermal gradient, it was found that in a Lorentz channel the Fourier law was satisfied, yet this system is not described by LTE. A modification of this model in which particles and scatterers can exchange energy through their collisions appeared in Ref. [11]. This effective interaction leads to the establishment of LTE. As a consequence, this model has proven to reproduce realistically macroscopic transport in many different situations [12]. In particular, the validity of the Fourier law was verified. One can conclude that, while the interaction among particles is not fundamental for the observation of normal transport, it is strictly necessary for the identification of microscopic dynamical quantities with the macroscopic physical parameters.

More recently, in order to investigate if chaos is a necessary condition for the validity



**FIGURE 1.** Geometry of different billiards: *a)* a Lorentz gas channel at critical horizon, *i.e.*, the separation among the centers of the discs is  $4R/\sqrt{3}$ , and *b)* a triangle billiard channel whose geometry is uniquely specified by assigning the internal angles  $\theta$  and  $\phi$ .

of Fourier law, a two-dimensional billiard model - which consists of a rectangular area and a series of triangular scatterers- was considered (see Fig. 1-*b*). This model is analogous to the Lorentz gas channel with triangles instead of discs, and the essential difference is that in the triangle billiard channel, the dynamical instability is linear; therefore the Lyapunov exponent is zero. Strong numerical evidence has been recently given [10] that the motion inside a triangle billiard, with all angles irrational with  $\pi$ , is mixing, without any time scale, (see also [19]). Moreover, an area-preserving map, which was derived as an approximation of the boundary map for the irrational triangle, shows a Gaussian diffusive behavior when considered on the cylinder, even though the Lyapunov exponent of the map is zero [9]. It is therefore reasonable to expect that the motion inside the irrational triangle billiard channel of Fig. 1-*b* is diffusive, thus leading to normal conductivity.

We have performed numerical simulations [20] on a triangle billiard channel of total length  $L = Nl$ , where  $N$  and  $l$  are the number and the length of the fundamental cells, as indicated in Fig 1. Heat baths have been simulated with stochastic kernels of Gaussian type: namely, the probability distribution of velocities for particles coming out from the baths is

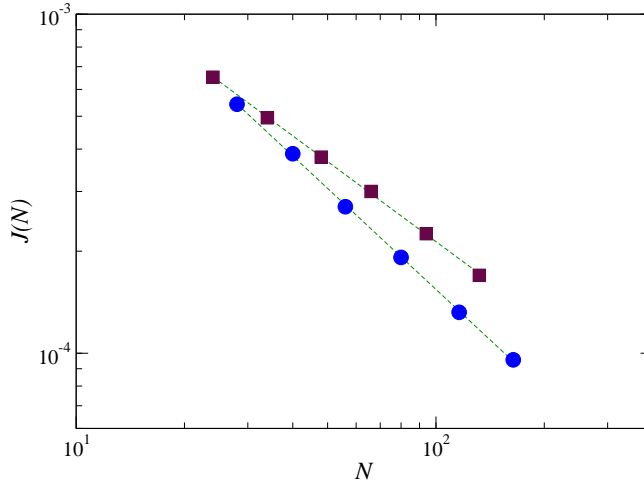
$$P(v_x) = \frac{|v_x|}{T} \exp\left(-\frac{v_x^2}{2T}\right), \quad P(v_y) = \frac{1}{\sqrt{2\pi T}} \exp\left(-\frac{v_y^2}{2T}\right) \quad (1)$$

for  $v_x$  and  $v_y$ , respectively. Since the energy changes only at collisions with the heat baths, the heat flux is given by

$$j(t_c) = \frac{1}{t_c} \sum_{k=1}^{N_c} (\Delta E)_k, \quad (2)$$

where  $(\Delta E)_k = E_{in} - E_{out}$  is the change in energy at the  $k$ th collision with the heat bath and  $N_c$  is the total number of such collisions that occur during time  $t_c$ .

In Fig. 2, the heat flux  $J$  as a function of the system size  $N$  is shown. For the case of irrational angles ( $\theta = (\sqrt{2} - 1)\pi/2$ ,  $\phi = 1$ ), the best fit gives  $J \propto N^{-\gamma}$ , with  $\gamma = 0.99 \pm 0.01$ . The coefficient of thermal conductivity is, therefore, independent on  $N$ , which means that the Fourier law is obeyed. The same result is obtained using the Green-Kubo formalism [20]. A completely different behavior is obtained when the angles  $\theta$  and



**FIGURE 2.** Scaling behavior of the stationary heat flux  $J$  as a function of the system size for the case of irrational angles of Fig. 1 (circles) and for the rational case (squares).  $N$  is the number of fundamental cells. The particle density was set to 1 particle per cell independently of  $N$ . The least-squares fitting gives a slope  $-0.99 \pm 0.01$  for the irrational case and  $-0.78 \pm 0.01$  for the rational one.

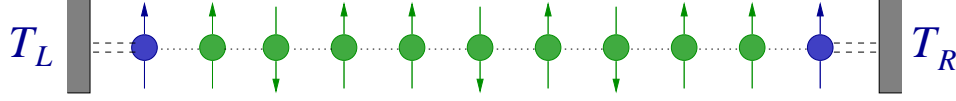
$\phi$  are rational multiples of  $\pi$ . The case with  $\theta = \pi/5$  and  $\phi = \pi/3$  is shown in Fig. 2 (triangles), from which a divergent behavior of the coefficient of thermal conductivity,  $\kappa \sim N^{0.22}$ , is observed, indicating the absence of the Fourier law.

In conclusion, when all angles are irrational multiples of  $\pi$ , the triangle billiard channel exhibits the Fourier law of heat conduction together with nice diffusive properties. However, when all angles are rational multiple of  $\pi$ , the model shows abnormal diffusion and the heat conduction does not follow the Fourier law.

One may argue that the model considered here is somehow artificial and far from a realistic physical model. Indeed, noninteracting particles systems are certainly less realistic as, in general, LTE is not established. In order to elucidate the role of interactions, we have studied in [21] and in [22] the so-called *1d hard-point particles with alternating masses* with and without total momentum conservation respectively. This model, consists of a one-dimensional chain of elastically colliding free particles with alternate masses  $m$  and  $M$  [6, 7]. It shares with the triangle billiard the linear dynamical instability but in contrast, it is a genuinely interacting many-particle system.

When the total momentum is conserved we have found that the heat current scales as  $J \propto N^{-\alpha}$  with  $\alpha \sim 0.745$  and thus, in contrast with the irrational triangle channel, the alternating mass model with conservation of total momentum does not obey the Fourier law [21]. We recall that in several recent papers [6, 23, 24] it has been suggested that total momentum conservation does not allow Fourier law and this may explain the lack of Fourier law for the one dimensional alternating mass model. Indeed, in [22] we have found that the alternate mass hard-point gas without total momentum conservation obeys the Fourier law.

In perspective, these results demonstrate that diffusive energy transport and Fourier law can take place in marginally stable (non-chaotic) interacting many-particles systems. As a consequence, the exponential instability (Lyapunov chaos) is not necessary for



**FIGURE 3.** Schematic representation of a finite one-dimensional quantum spin chain, coupled to external heat reservoirs at different temperatures.

the establishment of the Fourier law. Furthermore, our results show that breaking total momentum conservation is crucial for the validity of Fourier law.

### Fourier Law in Quantum Systems

In the previous section, we have shown that strong, exponentially unstable, classical chaos is not necessary (actually, strictly speaking, is not even sufficient [5]) for normal transport. In this connection we remark that a main feature of quantum motion is the lack of exponential dynamical instability [10]. Thus, it is interesting to inquire if, and under what conditions, the Fourier law emerges from the laws of quantum mechanics.

To this end we consider an Ising chain of  $L$  spins  $1/2$  with a coupling constant  $Q$  subject to a uniform magnetic field  $\vec{h} = (h_x, 0, h_z)$ , with open boundaries. The Hamiltonian reads

$$\mathcal{H} = -Q \sum_{n=0}^{L-2} \sigma_n^z \sigma_{n+1}^z + \vec{h} \cdot \sum_{n=0}^{L-1} \vec{\sigma}_n, \quad (3)$$

where the operators  $\vec{\sigma}_n = (\sigma_n^x, \sigma_n^y, \sigma_n^z)$  are the Pauli matrices for the  $n$ th spin,  $n = 0, 1, \dots, L-1$ . We set the coupling constant  $Q = 2$ . A schematic representation of this model is shown in Fig. 3. In this system, the only trivial symmetry is a reflection symmetry,  $\vec{\sigma}_n \rightarrow \vec{\sigma}_{L-1-n}$ . Moreover, the direction of the magnetic field affects the qualitative behavior of the system: If  $h_z = 0$ , the Hamiltonian Eq. (3) corresponds to the Ising chain in a transversal magnetic field. In this case, the system is integrable as it can be mapped into a model of free fermions through standard Wigner-Jordan transformations. When  $h_z$  is increased from zero, the system is no longer integrable, and when  $h_z$  is of the same order of  $h_x$ , quantum chaos sets in, leading to a very complex structure of quantum states as well as to fluctuations in the spectrum that are statistically described by Random Matrix Theory (RMT) [16]. The system becomes again (nearly) integrable when  $h_z \gg h_x$ . Therefore, by choosing the direction of the external field, we can explore different regimes of quantum dynamics.

The transition to quantum chaos for this model has been studied in [15]. We consider three cases: (i) the *chaotic chain*  $\vec{h} = (3.375, 0, 2)$ , (ii) the *integrable chain*  $\vec{h} = (3.375, 0, 0)$ , and (iii) the *intermediate chain*  $\vec{h} = (7.875, 0, 2)$  which is neither chaotic nor integrable.

In Ref. [15] we have simulated the coupling of the spin chain with thermal baths, requiring that the state of the spin in contact with the bath is statistically determined by a Boltzmann distribution with parameter  $T$ . Our model for the reservoirs is analogous to the stochastic thermal reservoirs defined by Eqs. (1), thus, we call it a *quantum stochastic*

*reservoir*. In what follows we use units in which the Planck and the Boltzmann constants are set to unity,  $\hbar = k_B = 1$ .

The dynamics of the spins is obtained from the unitary evolution operator  $U(t) = \exp(-i\mathcal{H}t)$ . Additionally, the leftmost and the rightmost spins of the chain are coupled to quantum stochastic reservoirs at temperatures  $\beta_T^{-1}$  and  $\beta_R^{-1}$ , respectively. For the details of the quantum stochastic reservoir model we refer the reader to Ref. [15] and for a comparison with the solution of the quantum master equation in Lindblad form to [25].

In order to compute the energy profile, we write the Hamiltonian in Eq. (3) as

$$\mathcal{H} = \sum_{n=0}^{L-2} H_n + \frac{h}{2}(\sigma_\lambda + \sigma_\rho), \quad (4)$$

where  $\sigma_\lambda = \vec{h} \cdot \vec{\sigma}_0/h$ ,  $\sigma_\rho = \vec{h} \cdot \vec{\sigma}_{L-1}/h$  are boundary terms and

$$H_n = -Q\sigma_n^z\sigma_{n+1}^z + \frac{\vec{h}}{2} \cdot (\vec{\sigma}_n + \vec{\sigma}_{n+1}), \quad 0 < n < L-2, \quad (5)$$

are the local energy density operators for the  $n$ th and  $(n+1)$ th spins.

The local current operators are defined through the equation of continuity:  $\partial_t H_n = i[\mathcal{H}, H_n] = -(J_{n+1} - J_n)$ , requiring that  $J_n = [H_n, H_{n-1}]$ . With Eqs. (5) and (4) the local current operators are explicitly given by

$$J_n = h_x Q (\sigma_{n-1}^z - \sigma_{n+1}^z) \sigma_n^y, \quad 1 \leq n \leq L-2. \quad (6)$$

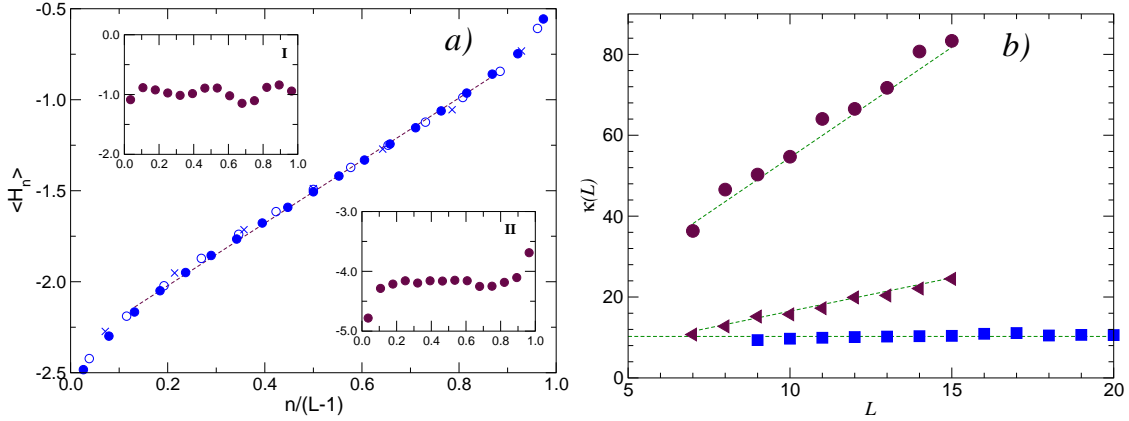
In Fig. 4-a, the energy profile for an out-of-equilibrium simulation of the chaotic chain is shown. After an appropriate scaling, the profiles for different sizes collapse to the same curve which is, to a very good approximation, linear. In contrast, in the case of the integrable (inset I) and the intermediate (inset II) chains, no energy gradient is created. In Fig. 4-b, the heat conductivity  $\kappa = J/\nabla(1/T)$  is shown as a function of the size of the chain. The constant value of  $\kappa$  for the chaotic spin chain indicates that the Fourier law is satisfied, while it is violated for the integrable and intermediate chains.

In conclusion these results suggest that the onset of quantum chaos is required for the validity of the Fourier law.

## THERMAL RECTIFICATION

We now turn our attention to the possibility of controlling the heat flow. Consider a system subjected to an external temperature gradient  $\nabla T$ , so that a stationary and uniform heat current  $J^+$  appears, transporting heat from the hot to the cold reservoir. Then consider the case in which the temperature gradient is inverted to  $-\nabla T$  and the heat current  $J^-$  is measured. In short, we say that the system is a thermal rectifier if  $J^+ \neq J^-$ . To quantify the power of rectification we use the ratio of the two currents:

$$\Delta = \frac{\max\{|J^+|, |J^-|\}}{\min\{|J^+|, |J^-|\}}. \quad (7)$$



**FIGURE 4.** *a)* Energy profile  $\langle H_n \rangle$  for the chaotic chain. The temperatures of the baths were set to  $T_L = 5$  and  $T_R = 50$ . Results for chains of size  $L = 8$  (crosses),  $L = 14$  (open circles) and  $L = 20$  (solid circles) are shown. The dashed line was obtained from a linear fit of the data for  $L = 20$  for the  $L - 4$  central spins. Insets (I) and (II) show the energy profiles for the integrable and the intermediate cases, respectively, for  $L = 15$ . *b)* Heat conductivity as a function of the system size for the chaotic (squares), integrable (triangles) and intermediate (circles) chains.

In Ref. [26] a microscopic mechanism for thermal rectification was proposed for the first time. There, an anharmonically interacting particles chain has been considered. Using an effective phonon approach, it was shown that by setting a strongly nonlinear central region sandwiched between two weakly anharmonic left and right domains, the anharmonic chain exhibits thermal rectification with ratio  $\Delta \sim 2$ . In [26] the phenomenon was explained in terms of the (non)matching of the effective phonon bands.

This and related ideas were further elaborated and improved [27, 28], achieving rectification efficiencies up to  $\Delta \sim 2000$ . Recently, the ideas in [27] have led to an interesting experimental work in which, thermal rectification has been observed [29]. A further step to devise a thermal transistor was discussed in [30] in terms of the negative differential thermal resistance observed in some anharmonic chains.

Other different mechanisms leading to thermal rectification have been described [31, 32]. In particular, in [32] thermal rectification in asymmetric billiards of interacting particles was described for the first time, and rectifications as large as  $\Delta \sim 10^3$  were observed. A simple phenomenological mechanism of thermal rectification, has also been recently discussed [33].

The possibility of obtaining large  $\Delta$  in billiard systems has raised great interest because they are more easily realizable experimentally in the rapidly expanding field of nanophysics. More recently we have proposed a novel mechanism for thermal rectification that results from the asymmetric behavior of the dynamics at a magnetic interface [34].

Consider a gas of noninteracting point particles of mass  $m$  and electric charge  $e$  that move freely inside a closed two-dimensional billiard region. The billiard has the geometry of the Lorentz gas channel of Fig. 1-a. Furthermore, we break the symmetry by considering that the left half of the billiard contains no magnetic field, whereas the right cell is subjected to a perpendicular uniform magnetic field of strength  $B$ . Finally,

the left and right boundaries of the billiard are coupled to stochastic heat baths (as in Eq. (1)), at temperatures  $T_L$  and  $T_R$ . A schematic representation of the billiard is shown in the inset of Fig. 5.

It is worth mentioning that the appearance of rectification does not depend on the particular geometry of the billiard. However, the negative curvature of the billiard boundary ensures that the motion in the absence of the magnetic field is completely chaotic.

The transmission probability between the left and right cells is controlled by the strength of the magnetic field. Consider the particles that cross the junction from *left to right*. There exist a critical velocity  $v_c$ : fast particles of velocity  $v > v_c$ , always enter the right cell, and thus contribute to the left to right energy flow provided they reach the right end of the system. Instead, slow particles of velocity  $v < v_c$ , such that the gyro-magnetic radius  $\rho(v) = mv/(eB)$  is less than  $\lambda/2$  will be reflected or transmitted depending on the position at which they reach the interface.

Using a statistical ensemble of trajectories, the condition for the critical velocity  $\rho(v_c) = \lambda/2$  can be rewritten as the condition giving a critical temperature

$$T_c = \frac{(eB_c\lambda)^2}{8mk_B}, \quad (8)$$

such that particles which are colder than  $T_c$  will be reflected in their majority.

In contrast, for the particles that cross the junction from *right to left* there is no condition on their velocity and they always enter the left cell. The above qualitative argument makes it clear that the transport of heat will be strongly asymmetric with respect to exchange of effective temperatures of particles on different sides of magnetic field boundary, provided the temperatures are strongly different, one being larger and the other smaller than  $T_c$ . Denoting with  $\tau = T/T_c$  the temperature in units of  $T_c$ , it is then clear that rectification will be effective if one of the temperatures is very small, say  $\tau_L \ll 1$  and the other is simply above the critical  $\tau_R > 1$ .

We measure the heat current per particle in the steady state as the time average of the energy transported across the junction per unit time

$$J = \lim_{t \rightarrow \infty} \frac{1}{t} \int_0^t \frac{1}{N} \sum_{i=1}^N E_i(s) \text{sgn}(v_{x,i}(s)) \delta(x_i - x_{\text{junc}}) ds, \quad (9)$$

where  $E_i(t) = \frac{1}{2}mv_i^2(t)$  is the instantaneous kinetic energy of the  $i$ th particle and  $x_{\text{junc}}$  the position along the  $x$ -axis of the junction. Furthermore, we denote the heat current as  $J^+$  if  $\tau_L < \tau_R$  and as  $J^-$  if the temperatures are exchanged, i.e.  $\tau_L > \tau_R$ .

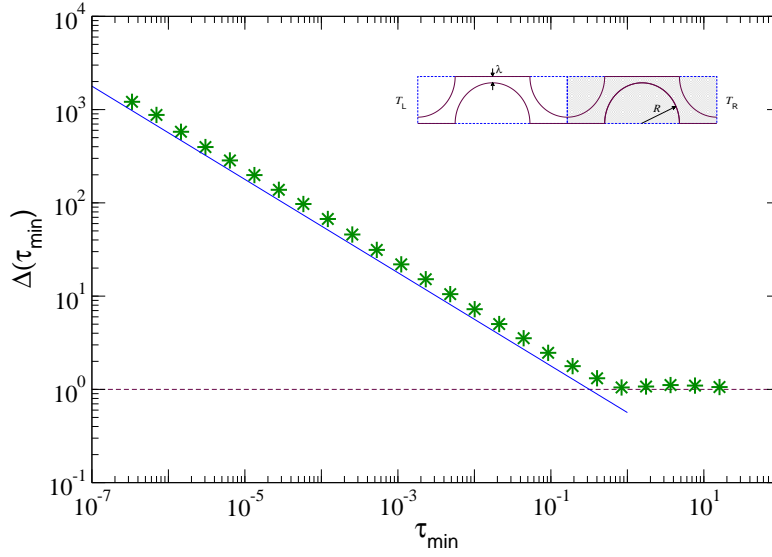
In [34] it was shown that, if  $\tau_L < \tau_R$ , the current  $J^+$  is proportional to the transmission coefficient at the interface  $t^+$  and invoking ergodicity, it can be estimated as  $t^+ \sim \frac{2\rho(v)}{\lambda}$ , where  $\rho(v(\tau)) = \sqrt{2mk_B\tau_{\min}}/eB$  and  $\tau_{\min} = \min\{\tau_L, \tau_R\}$ .

However, in the reverse situation (exchanging  $\tau_L$  and  $\tau_R$ ) we have  $t^- \sim 1$ , so the rectification becomes

$$\Delta = t^-/t^+ \propto \frac{1}{\sqrt{\tau_{\min}}}. \quad (10)$$

In Fig. 5 the rectification  $\Delta$  is shown as a function of  $\tau_{\min}$  for fixed value of the maximal temperature  $\tau_{\max}$ , confirming the estimate of Eq. (10). The correctness of the





**FIGURE 5.** Thermal rectification  $\Delta$  as a function of the minimal temperature  $\tau_{\min}$ . The maximal temperature was set to  $\tau_{\max} = 33.4275$ . The dashed line is for the no rectification value  $\Delta = 1$ . The solid line corresponds to  $\tau_{\min}^{-1/2}$ . Inset: schematic representation of the thermal rectifier.

scaling (10) shows that the magnetically induced rectification power is arbitrarily large for sufficiently small temperature  $\tau_{\min}$ .

## CONCLUSIONS

We have discussed the problem of heat conduction in classical and quantum low-dimensional systems. At the classical level, convincing numerical evidence exists for the validity of the Fourier law of heat conduction in linear mixing systems, *i.e.*, in systems without exponential instability. As a consequence, the exponential instability (Lyapunov chaos) is not necessary for the establishment of the Fourier law. Moreover, breaking total momentum conservation is crucial for the validity of the Fourier law while, somehow surprisingly, a less important role seems to be played by the degree of dynamical chaos.

At the quantum level, where the motion is characterized by the lack of exponential dynamical instability, we have shown that the Fourier law of heat conduction can be derived from a pure quantum dynamical evolution without any additional statistical assumptions. Similarly to our observations in classical models, our results for a chain of interacting spins suggest that in quantum mechanics, which is characterized by the lack of exponential dynamical instability, the onset of quantum chaos is required for the validity of the Fourier law.

We have also discussed the phenomenon of thermal rectification in different classical models and discussed different types of microscopic classical mechanisms that lead to rectification of heat flow. We have focused on the magnetically-induced thermal rectification and showed that for this mechanism, the rectification ratio  $\Delta$  is arbitrarily large for sufficiently small temperature of one of the heat baths. Present days nano-scale

experiments with meso-scopic devices should allow implementation of our theoretical model.

## ACKNOWLEDGMENTS

We gratefully acknowledge support by the MIUR-PRIN 2005 “Quantum computation with trapped particle arrays, neutral and charged”. C. M.-M. acknowledges a Lagrange fellowship from the Institute for Scientific Interchange Foundation.

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